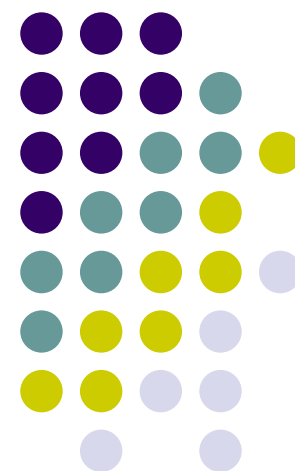


# An Informatics System for Service Life Prediction Data

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Joannie W. Chin  
Polymeric Materials Group  
May 17-18, 2006



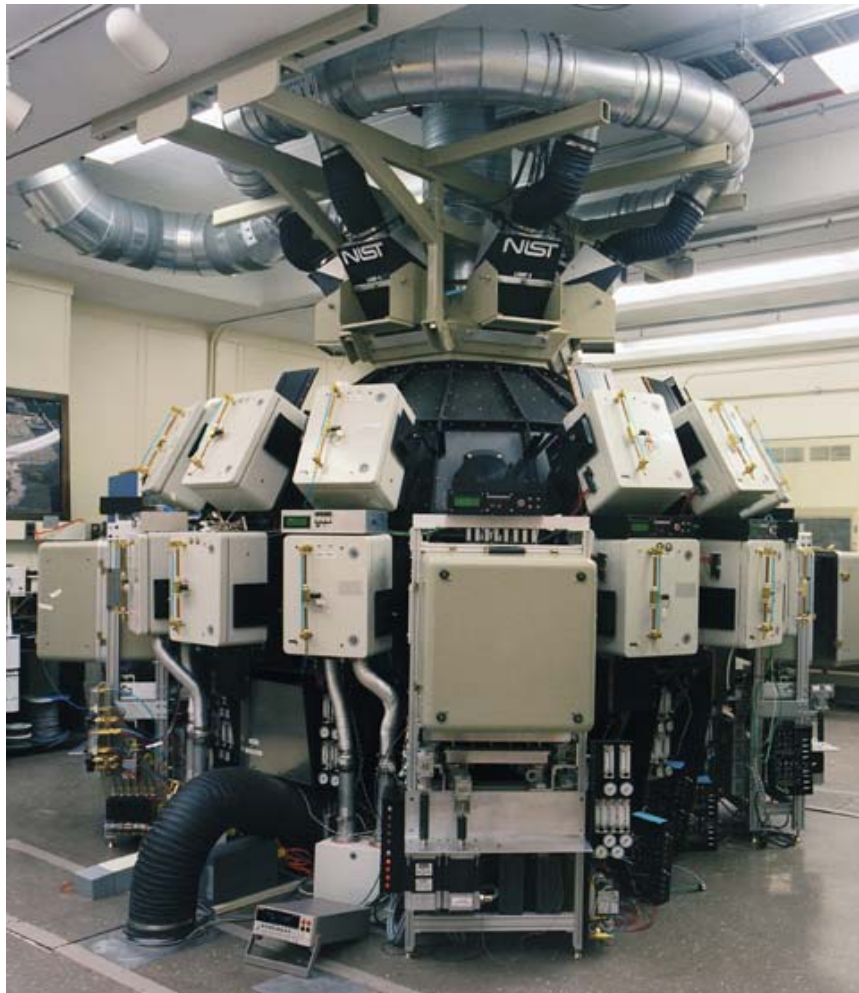
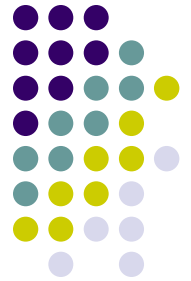


17 specimens/port

Typically, 50 measurement  
sets/experiment

> 160,000 data files per experiment!

# High Throughput UV Exposure



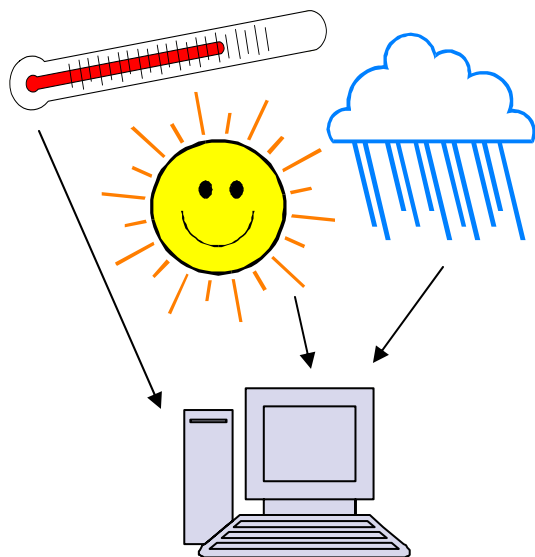
## During an experiment:

**Temperature\***,  
**relative humidity\***  
**flow controllers\***, and  
**shutter status**  
are automatically  
monitored and recorded  
every **6 minutes**  
for each of **32 ports**.

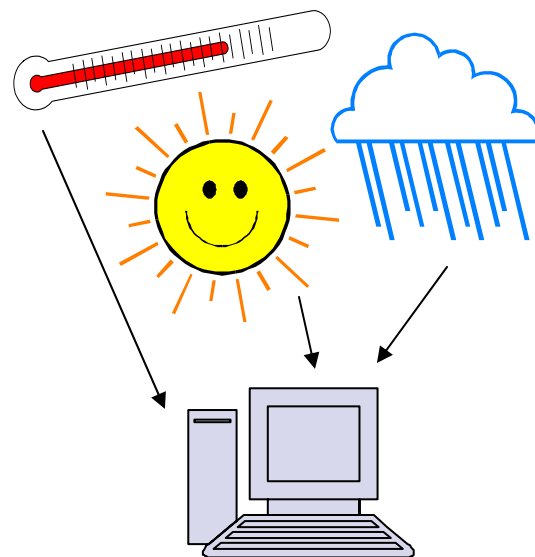
\* 8 sensors per port



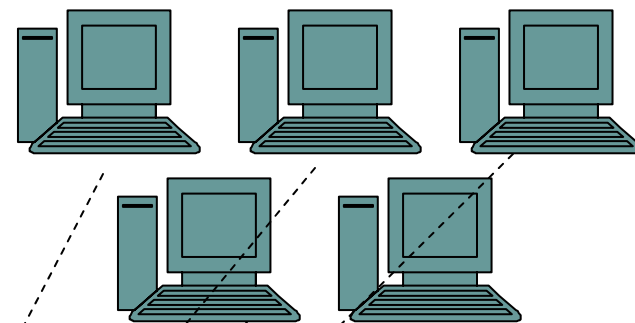
## Outdoor Environment



## Laboratory Environment



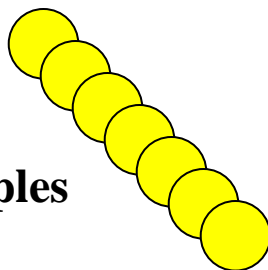
## Analytical Instruments



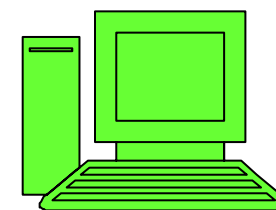
**Conventional**



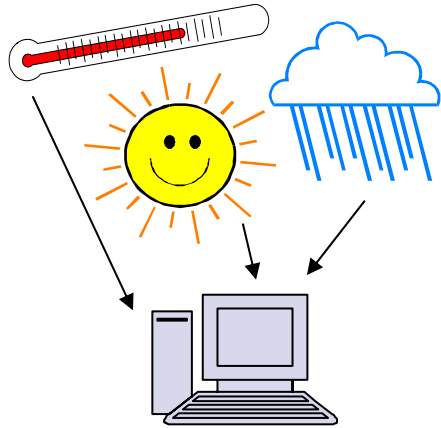
**Samples**



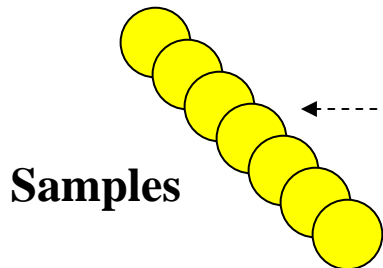
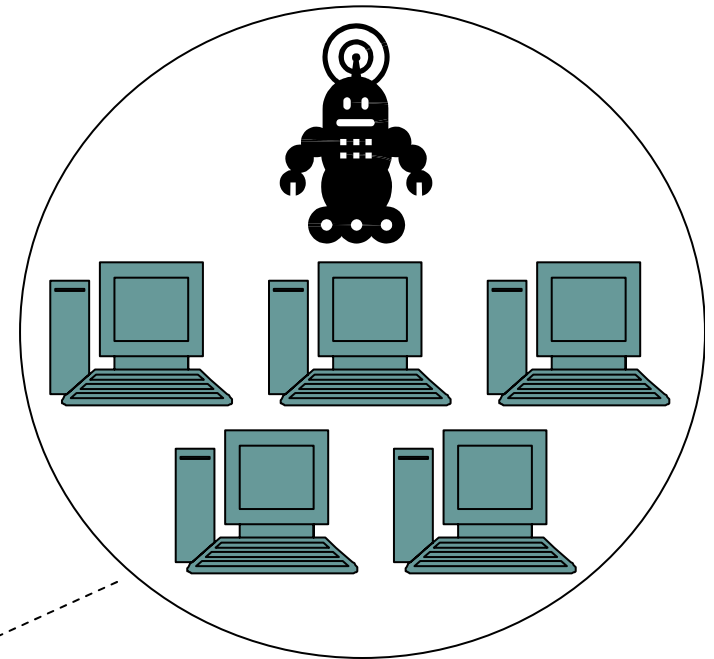
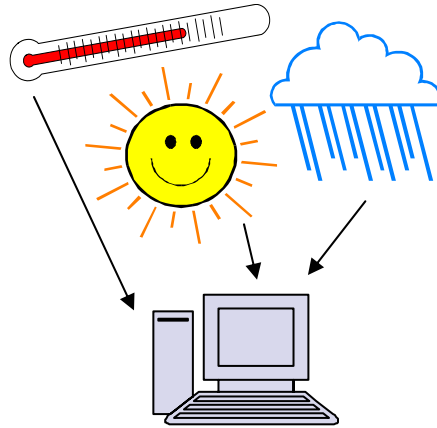
**User**



**Outdoor  
Environment**



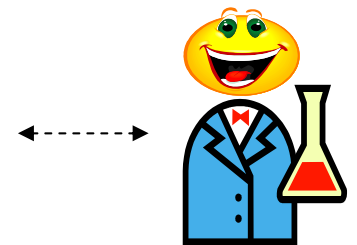
**Laboratory  
Environment**



**Samples**

**DATA BASE**

**DATA RETRIEVAL &  
PROCESSING  
PROGRAMS**



**Informatics**

- Based on *Firebird*, an open source database management system
- Multi-user architecture
- Unlimited capacity for data files
- Data format currently jcamp, eventually xml
- Contains sample information, analytical data and logs of environmental conditions



**DATA BASE**

Port	Assigned To	Status	Port Configuration
<a href="#">E01</a>	Debbie	Reserved	CaF
<a href="#">E02</a>	Debbie	Reserved	CaF
<a href="#">E03</a>	Chris	Under Construction	Mechanical
<a href="#">E04</a>	Debbie	In Use	CaF
<a href="#">E05</a>	Atlas - Debbie	In Use	CaF
<a href="#">E06</a>	Debbie	In Use	CaF
<a href="#">E07</a>	Chris	Under Construction	Mechanical
<a href="#">E08</a>	Debbie	In Use	CaF
<a href="#">E09</a>	Debbie	In Use	CaF
<a href="#">E10</a>	Debbie	In Use	CaF
<a href="#">E11</a>	Chris	Under Construction	Mechanical
<a href="#">E12</a>	Debbie	In Use	CaF
<a href="#">E13</a>	(currently occupied by Chris)	In Use	CaF
<a href="#">E14</a>	Joannie	In Use	CaF
<a href="#">E15</a>	Chris	Under Construction	Mechanical
<a href="#">E16</a>	Atofina (currently occupied by Chris)	In Use	CaF

Port	Assigned To	Status	Port Configuration
<a href="#">N01</a>	Debbie	Reserved	CaF
<a href="#">N02</a>	Debbie	Reserved	CaF
<a href="#">N03</a>	Stephanie	In Use	CaF
<a href="#">N04</a>	Debbie	In Use	CaF
<a href="#">N05</a>	Joannie	In Use	CaF
<a href="#">N06</a>	Debbie	In Use	CaF
<a href="#">N07</a>	Stephanie	In Use	CaF
<a href="#">N08</a>	Debbie	In Use	CaF
<a href="#">N09</a>	Debbie	In Use	CaF
<a href="#">N10</a>	Debbie	In Use	CaF
<a href="#">N11</a>	Stephanie	In Use	CaF
<a href="#">N12</a>	Debbie	In Use	CaF
<a href="#">N13</a>	Atlas - Debbie	In Use	CaF
<a href="#">N14</a>	Joannie	In Use	CaF
<a href="#">N15</a>	Stephanie	In Use	CaF
<a href="#">N16</a>	Atofina (currently occupied by Chris)	In Use	CaF

Status
In Use
Ready to Use
Under Construction
Reserved

Port Configuration
Configured for CaF Sample Holders
Configured for Mechanical Testing
No current configuration

## Port E10 4/21/2006 4:32:55 PM

Station status	
Operator	Debbie Stanley
Title	10 bottom
Specimen wheel ID	sample 1
Filter wheel ID	Filter wheel ID station 10 bottom
Cell ID	E10
Controlling	No
Temperature is	Not in spec
RH is	Not in spec
Shutter shows closed	
Shutter is set to close	
Door	closed
Shutter can	close
Temperature reading	OK
RH reading	OK
Alarm Status	No alarms
Master Reset	no
Micro	OK
Normal RH/T cell	
Dry Air Flow	0
Wet Air Flow	0
Data saved at 4/1/2006 12:00:04 AM	

Parameters for station 10				
	Target	Actual 1	Actual 2	Tolerance
Cell RH	75.0%	2.1%	2.3%	3.0%
Cell T	55.0C	26.8C	26.7C	1.5C
Tank T	57.0C	27.4C		
Air T	27.5C			

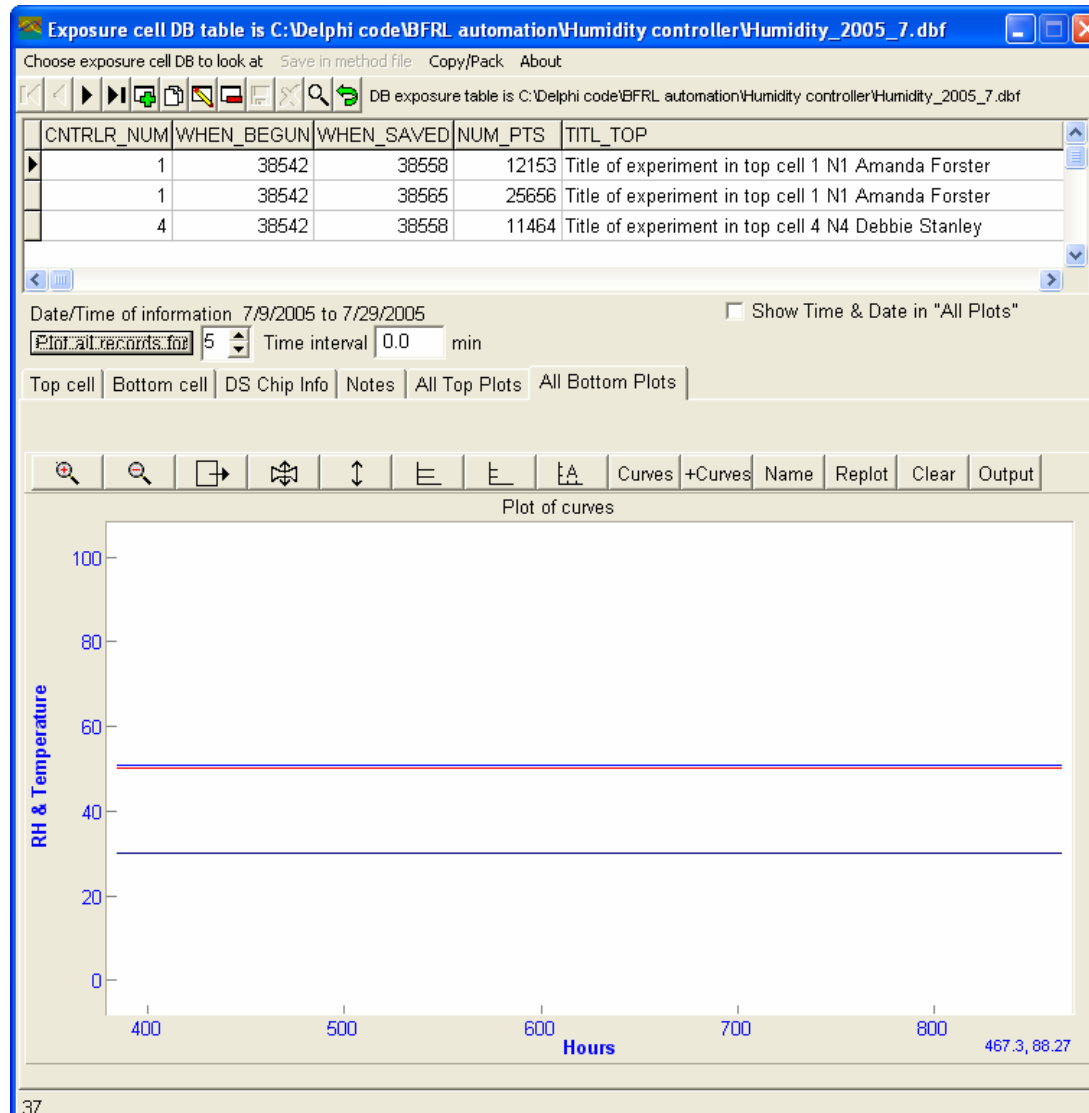
PID Parameters for station 10			
	PID 1	PID 2	PID 3
Cell	10	20	100
Air	15	20	100
RH	100	25	80

Caution - this page does not automatically update, you have to re-read it.

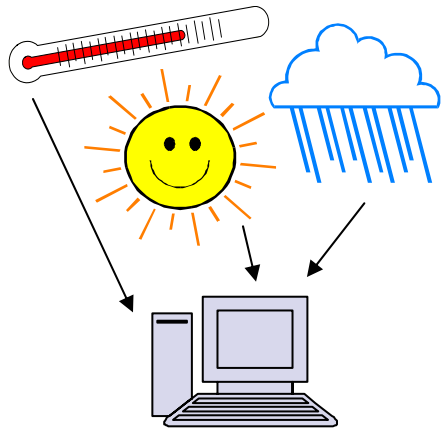
The data are updated about every 15 minutes.



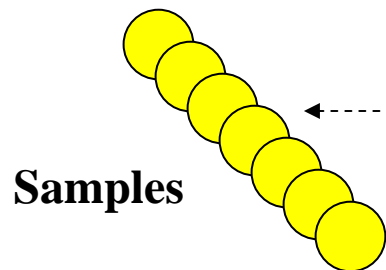
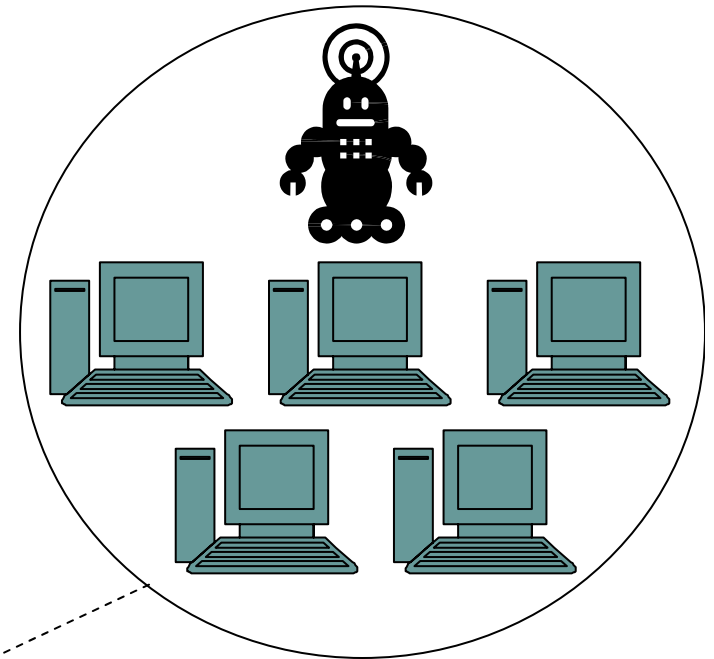
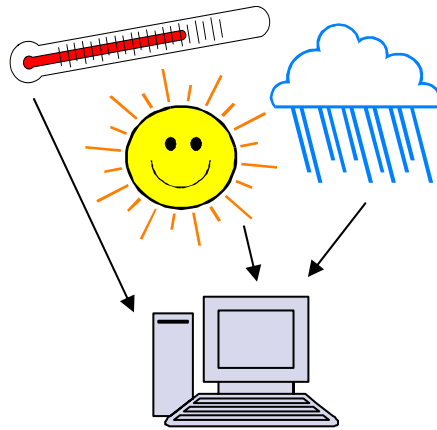
# Log of Experimental Conditions



**Outdoor  
Environment**

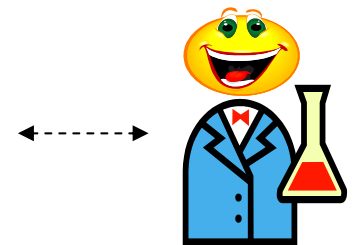


**Laboratory  
Environment**



**DATA BASE**

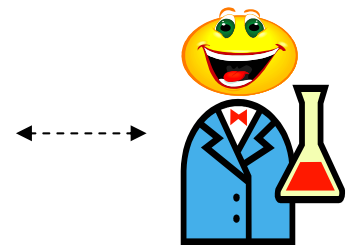
**DATA RETRIEVAL &  
PROCESSING  
PROGRAMS**



**Informatics**

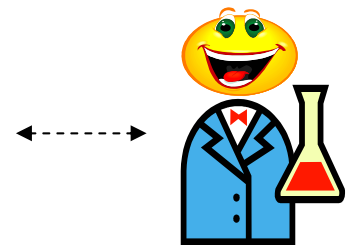
- Secure access and password protected
- Experimental matrix design program
- Calculation of damage/dosage data for exposed specimens

**DATA RETRIEVAL &  
PROCESSING  
PROGRAMS**



- Secure access and password protected
- **Experimental matrix design program**
- Calculation of damage/dosage data for exposed specimens

**DATA RETRIEVAL &  
PROCESSING  
PROGRAMS**



# Experimental Matrix Design Program

## Start Page



**BFRL SLP Exposure Program v1.14.0.1**

Measurement Details | Exptal Conditions | Report | Tables 1 | Tables 2 | Tables 3

Project Name: test with T/RH program

Material ID: Epoxy

Supplier:

Techniques

Spacing of measurements in days: 3

☒ Geometric measurement time intervals to skip

☒ IR transmission spectra

☒ UV transmission spectra

☒ Lamp intensity spectra

☒ Filter transmission spectra

☐ IR ATR spectra

☐ IR diffuse spectra

☐ Gloss

☐ TBA

☐ TBA

☐ TBA

Personnel

Project leader: Joannie Chin

Coworkers: Amanda Forster

Experiment Operator: Debbie Stanley



# Experimental Matrix Design Program

## Design Details



**BFRL SLP Exposure Program v1.14.0.1**

Measurement Details | Exptal Conditions | Report | Tables 1 | Tables 2 | Tables 3

Light Days at T/RH condition(s) in table or program (0 = do not use this condition)

RH/T	0%	25%	50%	75%
30C	100.0	0.0	0.0	100.0
40C	0.0	0.0	0.0	0.0
50C	0.0	0.0	0.0	0.0
60C	100.0	0.0	0.0	100.0

Number of replicates (0 = do not use this condition) for each filter condition

ND/WL	10 %	40 %	60 %	100 %
0	0	0	0	4
306 nm	0	0	0	4
326 nm	0	0	0	4
353 nm	0	0	0	4
452 nm	0	0	0	4

Specimen wheel priority for T/RH conditions

RH/T	0%	25%	50%	75%
30C	4	8	6	2
40C	14	10	15	11
50C	16	12	13	9
60C	3	7	5	1

Days in dark at T/RH conditions in table (0=do not use this condition)

RH/T	0%	25%	50%	75%
30C	0.0	0.0	0.0	0.0
40C	0.0	0.0	0.0	0.0
50C	0.0	0.0	0.0	0.0
60C	0.0	0.0	0.0	3000.0

T/RH Program 1

Hours	Deg C	%RH	Light?
5.00	35.0	70.0	y
10.00	45.0	50.0	y
15.00	55.0	30.0	n
20.00	45.0	50.0	y
25.00	35.0	70.0	y

Re-Initialise Tables, etc.

Change times: 200 days

Put In All: 4 reps

Efficiency of use of sphere: 0.670

# specimens in specimen wheel: 17

Clear Program Table ☐ Use Filter Matrix

# Replicates: 4 Total # Days: 100

☒ Assign to specimen and filter wheels ☐ Use any free spaces in current wheels

☒ Allow for neutral density filters by making all exposures roughly equal dosage ☐ Assign parameters to Project DB Table

☒ Add No UV and Unfiltered Specimens to Each Wheel

Roof/Outside

Number of replicates (0 = do not use this condition) for each filter condition

When	East	South	West	North
Jan-Mar	0	150	0	0
Apr-Jun	0	150	0	0
July-Sep	0	150	0	0
Oct-Dec	0	150	0	0

# Outside Replicates: 4 ☐ Use filters

Outside Sites

- ☐ Edgewater, MD
- ☐ Florida
- ☒ NIST roof
- ☒ Phoenix, AZ

# Dark Replicates: 4 **Assign Specimens**

Progress



# Experimental Matrix Design Program

## Assign exposure location



**BFRL SLP Port Assignment Program v**

Cell to position table ☐ Filter Records Available ports

CELL_NUM	POSITION	SPEC_WHEEL	FILTER1	TEMPERAT	HUMIDITY	T_TOL	RH_TOL	SITE	E_PROGRAM	RH
NSS-0001	NSS1-N01	NSS-0001	NSF-0001	30	0	2	3	NSS1		(Me
NSS-0002	NSS1-N02	NSS-0002	NSF-0002	30	0	2	3	NSS1		(Me
NSS-0003	NSS1-N03	NSS-0003	NSF-0003	30	0	2	3	NSS1		(Me
NSS-0004	NSS1-N04	NSS-0004	NSF-0004	30	0	2	3	NSS1		(Me
NSS-0005	NSS1-N05	NSS-0005	NSF-0005	30	0	2	3	NSS1		(Me
NSS-0006		NSS-0006	NSF-0006	60	0	2	3	NSS1		(Me
NSS-0007		NSS-0007	NSF-0007	60	0	2	3	NSS1		(Me
NSS-0008		NSS-0008	NSF-0008	60	0	2	3	NSS1		(Me
NSS-0009		NSS-0009	NSF-0009	60	0	2	3	NSS1		(Me
NSS-0010		NSS-0010	NSF-0010	60	0	2	3	NSS1		(Me
NSS-0011		NSS-0011	NSF-0011	30	75	2	3	NSS1		(Me
NSS-0012		NSS-0012	NSF-0012	30	75	2	3	NSS1		(Me
NSS-0013		NSS-0013	NSF-0013	30	75	2	3	NSS1		(Me
NSS-0014		NSS-0014	NSF-0014	30	75	2	3	NSS1		(Me
NSS-0015		NSS-0015	NSF-0015	30	75	2	3	NSS1		(Me
NSS-0016		NSS-0016	NSF-0016	60	75	2	3	NSS1		(Me

Available ports: NSS1-E01, NSS1-E02, NSS1-E03, NSS1-E04, NSS1-E05, **NSS1-E06**, NSS1-E07

SPEC_NUM	FILT_NUM	CELL_NUM	WHEN
NSS-0001	NSF-0001	NSS-0001	38831.9709
NSS-0002	NSF-0002	NSS-0002	38831.9709
NSS-0003	NSF-0003	NSS-0003	38831.9709
NSS-0004	NSF-0004	NSS-0004	38831.9709
NSS-0005	NSF-0005	NSS-0005	38831.9709
NSS-0006	NSF-0006	NSS-0006	38831.9709

Specimen and filter wheels to cell table

TIME	FILT_WHEEL	HOLE_NO	FILTER_NO	DENSITY	IN_USE	PROJECT
38853.6007	NSF-0001	1	none	100	Y	Test Project
38853.6007	NSF-0001	2	none	100	Y	Test Project
38853.6007	NSF-0001	3	none	100	Y	Test Project
38853.6007	NSF-0001	4	none	100	Y	Test Project
0	NSF-0001	5		0	N	none
0	NSF-0001	6		0	N	none

Filter to filter wheel table



# Experimental Matrix Design Program

## T/RH Controllers and Robot read DB record



BFRL Humidity Controller, version 1.103.0.1

Ini Files Method File About

Select a controller: 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32

DB name goes here

Title Control History T Cell Program Graph Deltas Guess PIDs Error Msgs DB Tables Tables 2

**Control details**

Project Test Project Epoxy Joannie Chin Total exposure time 100 days Programmed 5/15/2006 6:51:24 PM  
 Specimen Wheel NSS-0005 Filter Wheel NSF-0005 Cell ID NSC-0005 Operator Debbie Stanley

	Target	Actual	Fluctuation	Slope	Baseline
%RH 1	0.0	0.0	0.0	0.0301	0.811
%RH 2		0.0	0.0	0.0309	0.823
Tolerance on RH	3.0				
Cell temperature 1	30.0	0.0	0.0		
Cell temperature 2		0.0	0.0		
Water tank temperature	30.0	0.0	0.0		
Chamber air temperature		0.0	0.0		
Tolerance on temperature	2.0				

**Cell PID parameters**

Proportional 1  
 Integral 10  
 Differential 100

**Chamber air PID parameters**

Proportional 1  
 Integral 10  
 Differential 50

**RH PID parameters**

Proportional 1  
 Integral 15  
 Differential 50

Get target values

Green = used in control  
 Red = control parameter  
 Blue = used to monitor

☒ Show any new data  
☒ Show target parameters Targets not updated Data not updated

Send to controller Time now 5/16/2006 1:36:36 PM

Targets Slopes & baselines PID parameters Parameters to Clipbd



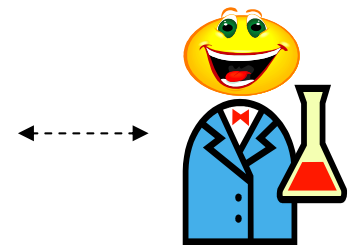


Robot Controller Program

- Secure access and password protected
- **Experimental matrix design program**
- Calculation of damage/dosage data for exposed specimens

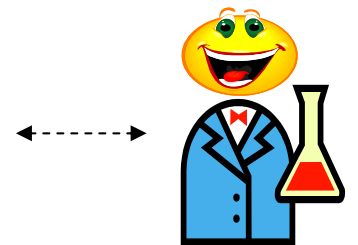
T/RH Controller

**DATA RETRIEVAL &  
PROCESSING  
PROGRAMS**



- Secure access and password protected
- Experimental matrix design program
- Calculation of damage/dosage data for exposed specimens

**DATA RETRIEVAL &  
PROCESSING  
PROGRAMS**



# Damage-Dosage Calculation Program



**Assess specimen damage from database files, version 3.98.0.1**

Specimen/Cell DB Tables | Specimen Dosage | Control IR Spectra | UV-IR Spectra | Dosage vs Damage | IR Spectra for Plates | Sliced Irradiance  
 Specimen Status | UV Tables after Query | Run Comments | Active DataBases | Specimen Graphs | Lamp and Filter Graphs | Diff UV & IR Correlations

Configuration file is C:\Documents and Settings\dstanley\Desktop\Programs\Brians Programs\New DATABASE files\Composite SLP data test.ini INI file Menu.... ▼

Active Databases - The Order of the Dbs follows the Light Path from Lamp to Specimen

**Lamp DBs**

Lamps On/Off DB table is C:\Documents and Settings\dstanley\Desktop\Programs\Brians Programs\New DATABASE files\A new Lamp On Off DB.dbf

Lamp Spectra DB table is C:\Documents and Settings\dstanley\Desktop\Programs\Brians Programs\New DATABASE files\LAMP INTENSITY.dbf

Position To Lamp Number DB table is \\Bfri-b325-scan\scanner\_drive\_f\SLP\_Data\Sphere Data Continued 2005-06-14\New Position To Lamp.dbf

Fiber Calibration DB table is \\Bfri-b325-scan\scanner\_drive\_f\SLP\_Data\Sphere Data Continued 2005-06-14\Fiber\_Power Scaled from 2 to 1 7 7 2005.DBF

Position to Fiber DB table is \\Bfri-b325-scan\scanner\_drive\_f\SLP\_Data\Sphere Data Continued 2005-06-14\Fiber\_Power Scaled from 2 to 1 7 7 2005.DBF

**Cell Contents (Filter, T and RH)**

Cell Position/Contents DB table is \\Bfri-b325-scan\scanner\_drive\_f\SLP\_Data\Sphere Data Continued 2005-06-14\New Cell Positions.dbf

Cell T and RH record

Filter Spectra DB table is C:\Documents and Settings\dstanley\Desktop\Programs\Brians Programs\New DATABASE files\FILTER SPECTRA.dbf

Filter IDs DB table is \\Bfri-b325-scan\scanner\_drive\_f\SLP\_Data\Sphere Data Continued 2005-06-14\Filter ID-ID.dbf

**Specimen DBs**

Specimen IDs DB table is \\Bfri-b325-scan\scanner\_drive\_f\SLP\_Data\Sphere Data Continued 2005-06-14\Specimen ID new fields all specimens indoor.dbf

Specimens In Cells DB table is \\Bfri-b325-scan\scanner\_drive\_f\SLP\_Data\Sphere Data Continued 2005-06-14\SPECIMENINCELLS.dbf

Specimen Spectra DB table is C:\Documents and Settings\dstanley\Desktop\Programs\Brians Programs\New DATABASE files\UV-VIS SAMPLE SPECTRA.dbf

Specimen IR Spectra DB table is C:\Documents and Settings\dstanley\Desktop\Programs\Brians Programs\New DATABASE files\IR SPECTRA.dbf

Specimen IR Substrate Spectra DB

Specimen UV-vis Substrate Spectra DB

**Damage DB**

Damage DB for Spectra of Specimens In Cells

1



# Damage-Dosage Calculation Program



**Assess specimen damage from database files, version 3.98.0.1**

Specimen/Cell DB Tables | Specimen Dosage | Control IR Spectra | UV-IR Spectra | Dosage vs Damage | IR Spectra for Plates | Sliced Irradiance

Specimen Status | UV Tables after Query | Run Comments | Active DataBases | Specimen Graphs | Lamp and Filter Graphs | Diff UV & IR Correlations

**Specimen Details**

About this Program | | Process this Specimen Manually

Now doing slice 17 for specimen NSS-0016-02 from 03/02/2006 at 07:44:58 PM to 03/02/2006 at 08:15:04 PM

Show Ablation Details  
Show Clipboard  
Clear All Plots

Specimen Number **NSS-0016-02**  
Specimen ID **BFRL epoxy on 19 mm dia 4 mm thin CaF2**  
Specimen source **BFRL**

Time limits for calculations  
Calculate exposure from **10/ 1/2005**  
Calculate exposure to **5/16/2006**  
☐ Ignore these times, do all of specimen

☐ Subtract substrate UV spectra  
☐ Subtract substrate IR spectra  
☒ UV-vis of thick specimen 0 scaled down by thickness  
☐ Get irradiance Pause time (s) **0.0**

Automatic processing  
☐ Add To Damage DB if Auto Mode ☐ Pause if Auto Mode  
Process automatically for next **1** specimens, 0= do all  
Do Specimens Automatically Stop Processing  
☐ Print Out Plots ☒ Don't clear plots  
☒ Auto rewinding DBs ☒ Do subset ☐ Write T/RH/Dosage File  
☒ Show error messages ☐ Outside Exposures  
☐ Use only good specimens ☐ Pause if Noisy

Subsets  
vL **353.00** Neutral Den **100.00** T **35.0** RH **50.0**

Searching Dbs...

Specimen Current Conditions  
Cell = NSC-0016-02 on 10/27/2005 Cell Temperature = 35.0C Cell Humidity = 50.0%RH Thickness = 5.4  
Filter = NSF-0016-02 Cell Filter vL = 353.00 Cell Filter Half Width = 19.00  
Number of cells for this specimen = 1 Cell position = NS1-E08 Control Specimen # = NSS-0016-01 No UV specimen # = NSS-0016-01  
Filter ND = 100.00% Filter ID Specs = 354nm, 24nm Bandpass + No Neutral Density Filter

Limits Defining Non-Zero Data  
Minimum "Significant" UV Absorbance in Filter Range **0.025** Minimum IR Absorbance Range **0.025** More than this fraction of sign reversals (+/-) will mean a curve is just noise **1.000**  
☐ Do Time Trends by Right-Clicking on Plots

Operate on Damage Plots  
Estimate specimen thickness/ablation in IR at **2960.000** Look for ablation site  
☐ If checked, click on IR will select new place to use to estimate ablation  
☐ Scale Ablation to Std Specimen Thickness ☒ Scale Data by Specimen Thickness  
Standard Thickness of Specimen in IR Units **6.000** ☒ Scale Data to Standard Thickness  
☒ Subtract Control Specimens ☐ Scale All IR Spectra To Control IR Spectra  
☐ Average all correlated damage sites

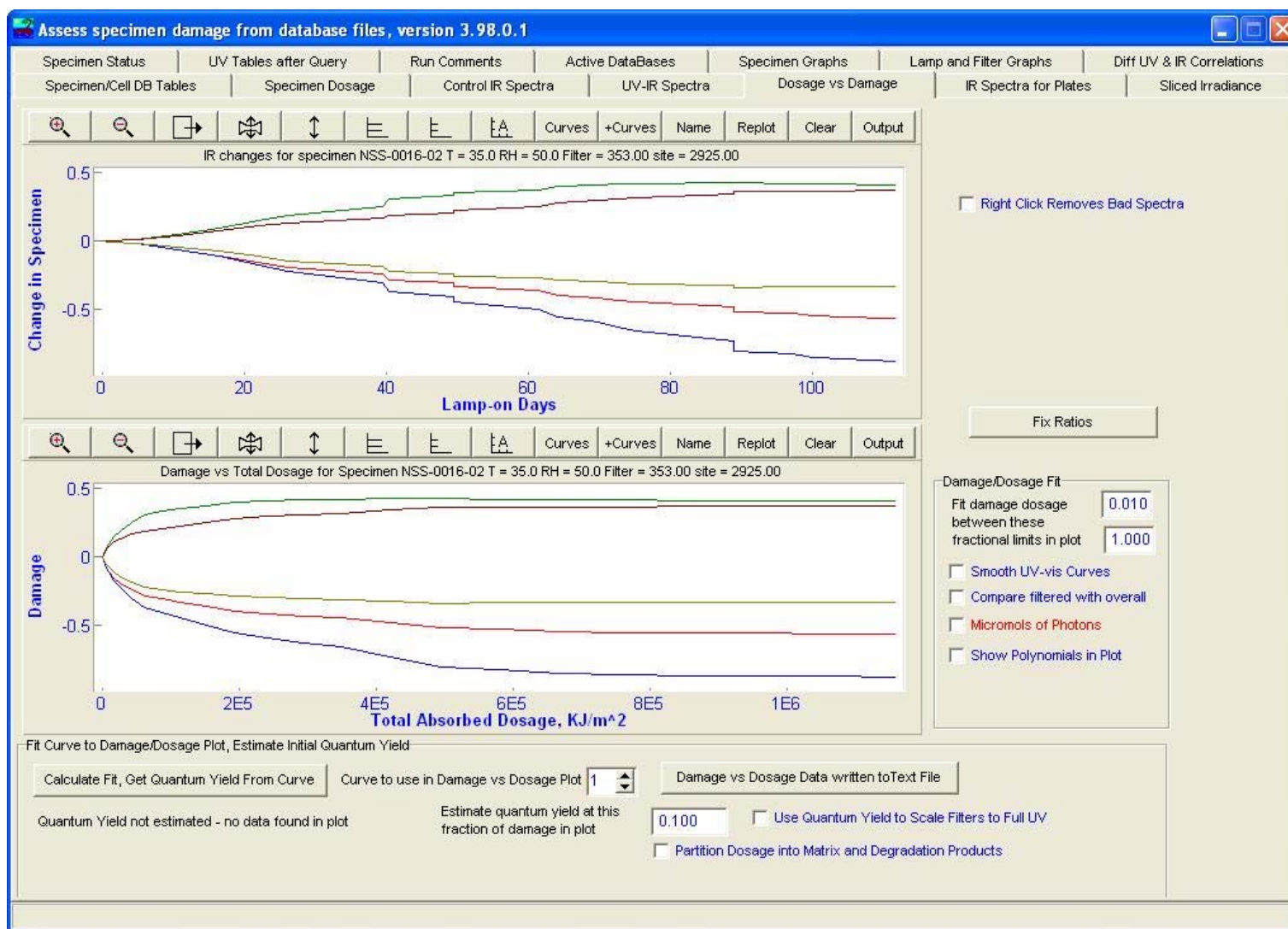
Set Control  
Set control to have filter max of **0.0**  
☐ Add Control Profiles to Damage Database Table

Zero Spectra at these Sites  
☐ Use Lamp Zero ☒ Use UV-vis Zero ☒ Get UV-vis Zero from thick specimen  
Zero lamp spectra at **200.0** Zero specimen UV-vis spectra at **800.0**

Do automatic processing for the number of specimens shown in the spin button (0=do all from the current specimen to the end of the DB)



# Damage-Dosage Calculation Program





# Gantt Chart



Y1

Y2

Y3

Y4

Link laboratory sensors to database (completed)

Convert data and image processing programs already being utilized in SLP research (completed)

Complete framework for database and populate with data files



Link outdoor sensors to main database



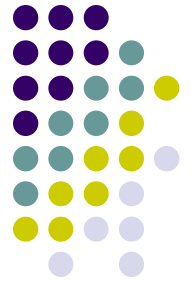
Establish automatic communication from instruments in high throughput analytical laboratory



Development of data “wizard” to detect and correct erroneous data



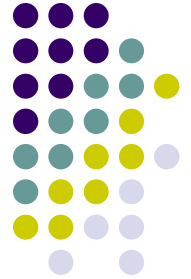
# Impacts



- **Key component** of service life prediction program, enhances the unique capabilities of the NIST SPHERE and associated devices.
- Ability to collect, store, and analyze large amounts of data in different formats from different instruments in an *automated* fashion, with greatly improved:
  - specimen characterization speed
  - data traceability and quality, reduction of user error
  - data retrieval and processing speed
- Informatics systems framework will serve as a model for any research programs that routinely generate large amounts of data.



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